Competing Supersolid and Haldane Insulator phases in the extended one-dimensional bosonic Hubbard model

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The Haldane Insulator is a gapped phase characterized by an exotic non-local order parameter. The parameter regimes at which it might exist, and how it competes with alternate types of order, such as supersolid order, are still incompletely understood. Using the Stochastic Green Function (SGF) quantum Monte Carlo (QMC) and the Density Matrix Renormalization Group (DMRG), we study numerically the ground state phase diagram of the one-dimensional bosonic Hubbard model (BHM) with contact and near neighbor repulsive interactions. We show that, depending on the ratio of the near neighbor to contact interactions, this model exhibits charge density waves (CDW), superfluid (SF), supersolid (SS) and the recently identified Haldane insulating (HI) phases. We show that the HI exists only at the tip of the unit filling CDW lobe and that there is a stable SS phase over a very wide range of parameters.

PACS numbers: 03.75.Hh 05.30.Rt 67.85.-d

Since its introduction in 1989 [1], the bosonic Hubbard model (BHM) has attracted continued interest due to its very rich ground state phase diagram especially in the presence of longer range interactions. Direct experimental relevance was established with the realization of this model Hamiltonian, with tunable parameters [2], in systems of ultra-cold bosonic atoms loaded in optical lattices [3]. In its simplest form, a single boson species with only contact repulsion, the system exhibits two phases in the ground state [1], a superfluid (SF) and an incompressible Mott insulator (MI) depending on the particle filling and the interaction strength. Extensive quantum Monte Carlo (QMC) simulations have established that, when longer range interactions are included, the supersolid (SS) phase can form for a wide range of parameters and lattice geometries in one, two and three dimensions [4–16]. Typically, the SS phase is produced by doping a phase exhibiting long range charge density order (CDW). However, further QMC work has shown that, remarkably, for a wide range of parameters, the extended BHM with near neighbor interactions exhibits a SS phase even at *commensurate* fillings in two and three dimensions [17, 18].

In addition, it was shown that the one-dimensional extended BHM with next near and/or near neighbor interactions admits another exotic phase at a filling of one particle per site; the Haldane insulator (HI) [19, 20]. The HI is a gapped insulating phase characterized by a highly non-local order parameter like the Haldane phase [21, 22] in integer spin chain systems (see below). This gives rise to several questions. Does the HI exist for other integer fillings of the system or is it a special property of the unit filling case? The SS phase found in one dimension [11] was obtained by doping a CDW phase: Does this phase also exist for commensurate fillings in one dimension for parameter choices similar to those in two [17] and three dimensions [18]? If the SS phase exists for commensurate fillings, where is it situated in the phase diagram relative to the CDW, MI and HI phases? The phase diagram at unit filling for the BHM with contact (U) and near neighbor (V) interactions was determined via QMC [23, 24] and found to have SF, MI and CDW phases but no SS. Subsequently, the (μ, t) phase diagram of the extended BHM, for a fixed V/U ratio, was obtained using Density Matrix Renormalization Group (DMRG) [25], but showed only evidence for MI, SF and CDW. More recent work, also based on the DMRG, has found [26] no SS phase in the (U, V) plane at unit filling but the question of other fillings was not addressed. Reference [26] also found a HI phase sandwiched between the MI and CDW phases which was not present in [23, 24]. As we shall see below, the HI phase was not found in the earlier work because the superfluid density in this phase vanishes very slowly with the system size and the largest sizes that could be accessed at the time were 64 sites.

Theoretical studies of this system using bosonization have led to mixed results. The HI was obtained and characterized with bosonization [20] but consensus is absent on whether the SS phase exists in this model. Even though older studies did not specifically mention it [27] or even argued that it did not exist [25], more recent studies seem to demonstrate the presence of the SS phase [28], even without nearest

neighbor interaction [29], for both commensurate and incommensurate fillings. However, the precise nature of order and the decays of the relevant correlation functions are still far from settled. For instance, some studies predict that the single particle Green function decays exponentially in the SS phase while the density-density correlation function decays as a power [30]; others predict that both of these correlation functions decay as powers [28]. Finally, the universality class of the transition to the SS phase remains largely unexplored.

In this Letter we answer some of these questions using the Stochastic Green Function (SGF) QMC algorithm [31] and the ALPS [32] DMRG code to obtain the phase diagram of the extended BHM in one dimension,

$$H = -t\sum_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \frac{U}{2}\sum_i n_i\,(n_i - 1) + V\sum_i n_i n_{i+1}. \qquad (1)$$

The sum over i extends over the L sites of the lattice, periodic boundary conditions were used in the QMC and open conditions with the DMRG. The hopping parameter, t, is put equal to unity and sets the energy scale, a_i ($a_i^\dagger$) destroys (creates) a boson on site i, $n_i = a_i^\dagger a_i$ is the number operator on site i, U and V are the onsite and near neighbor interaction parameters. All results presented here were obtained at the fixed ratio $V/U = 3/4$ which favors CDW phases over MI at commensurate fillings when U is large.

Several quantities are needed to characterize the phase diagram. The superfluid density is obtained with QMC using [33]

$$\rho_s = \frac{\langle W^2\rangle}{2td\beta L^{d-2}}, \qquad (2)$$

where W is the winding number of the boson world lines, d is the dimensionality and β the inverse temperature. The CDW order parameter is the structure factor, $S(k)$, at $k = \pi$ where

$$S(k) = \frac{1}{L}\sum_{r=0}^{L-1} \mathrm{e}^{ikr}\langle n_0 n_r\rangle, \qquad (3)$$

and the momentum distribution, n_k, is given by

$$n_k = \sum_{r=0}^{L-1} \mathrm{e}^{ikr}\langle a_0^\dagger a_r\rangle. \qquad (4)$$

The charge gap is given by $\Delta_c(n) = \mu(n) - \mu(n-1)$; the chemical potential is $\mu(n) = E_0(n+1) - E_0(n)$ where $E_0(n)$ is the ground state energy of the system with n particles and is obtained both with QMC and DMRG. The neutral gap, Δ_n, is obtained using DMRG by targeting the lowest excitation with the same number

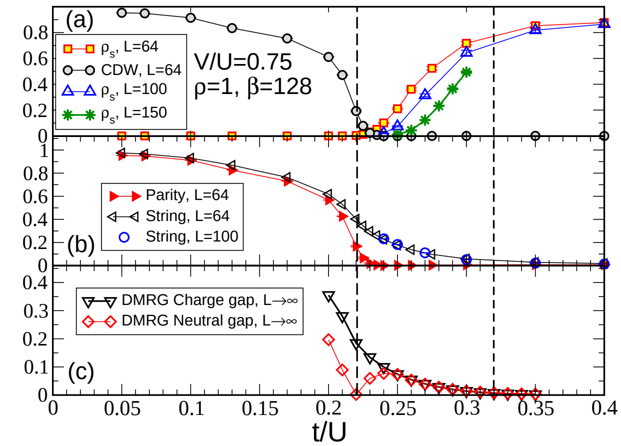

FIG. 1: (color online) Shows several quantities for $\rho = 1$ as functions of t/U with the fixed ratio $V/U = 0.75$. (a) The CDW order parameter for $L = 64$ and ρ_s for $L = 64$, 100, 150; (b) the parity and string order parameters; (c) the neutral and charge gaps. (a) and (b) were obtained with QMC and (c) with DMRG. The region between the vertical dashed lines is the HI. In the HI, $\rho_s \to 0$ very slowly as L increases while the string parameter is essentially constant. Note the difference between the neutral and charge gaps. The gaps are given in units of the hopping t.

of bosons. In both CDW and HI phases, the chemical potentials at both ends are set to (opposite) large enough values, in DMRG, such that the ground state degeneracy and the low energy edge excitations are lifted [19, 25]. With the SGF we did simulations in both the canonical and grand canonical ensembles.

For large values of U and V at $\rho = 1$, a site typically has $n_r = 0, 1, 2$ particles with higher occupations being very rare. The system then becomes analogous to an $S = 1$ spin chain [19] with $S_z(i) \equiv \delta n_i = n_i - \rho$ ($\rho = 1$ here) taking values of $0, \pm 1$. Consequently, string and parity operators can be defined [19, 20] to characterize the Haldane Insuating phase,

$$\mathcal{O}_s(|i-j|) = \langle \delta n_i \mathrm{e}^{i\theta\sum_{k=i}^{j}\delta n_k}\delta n_j\rangle, \qquad (5)$$

$$\mathcal{O}_p(|i-j|) = \langle \mathrm{e}^{i\theta\sum_{k=i}^{j}\delta n_k}\rangle, \qquad (6)$$

where $\theta = \pi$ for $S = 1$. The corresponding value of the order parameter is obtained in the limit $|i-j| \to \infty$; in practice we take the order parameters to be $\mathcal{O}_{s/p}(L_{max})$ where, in QMC with PBC, $L_{max} = L/2$ and in DMRG, with OBC, L_{max} is the longest distance possible before edge effects start being felt. For higher integer filling, $\rho = 2, 3\ldots$, $\theta \neq \pi$ and has to be determined as discussed in [34]. It was shown [19, 20] that the phases are characterized as follows [37]: In MI, $\rho_s = 0$, $S(\pi) = 0$, $\Delta_c = \Delta_n \neq 0$, $\mathcal{O}_p(L_{max}) \neq 0$, $\mathcal{O}_s(L_{max}) = 0$; in CDW,

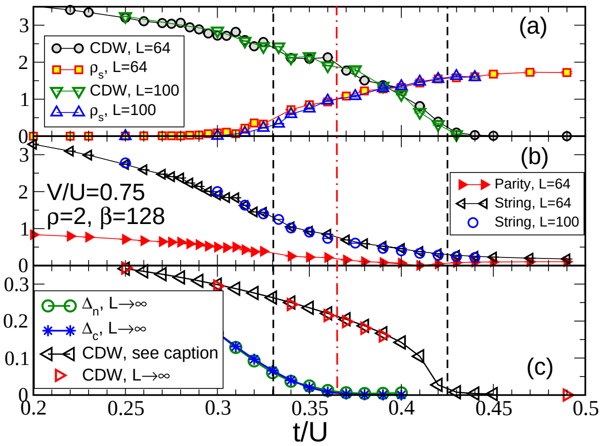

FIG. 2: (color online) Same as Fig. 1 but at $\rho = 2$. (a) QMC simulations show that in the interval between the two vertical (black) dashed lines there is similtaneous SF and CDW order and, therefore, a supersolid phase (SS). The vertical (red) dot-dash line is where the $L \to \infty$ extrapolated neutral (Δ_n) and charge (Δ_c) gaps vanish in DMRG (c). The CDW-SS transition is between $t/U = 0.33$ (QMC) and $t/U = 0.355$ (DMRG). The difference between the two values could be due to the difference in the boundary conditions, open for DMRG and periodic for QMC. (c) also shows the $L \to \infty$ extrapolated CDW order parameter, right (red) triangles, and the Fourier transform of $\langle n_i \rangle \langle n_j \rangle$, left (black) triangles, obtained with DMRG to probe the disappearance of CDW order. Both DMRG and QMC give the SS-SF transition at $t/U \approx 0.425$. Note that, unlike Fig. 1, the charge and neutral gaps (c) are essentially always the same.

$\rho_s = 0$, $S(\pi) \neq 0$, Δ_c and $\Delta_n \neq 0$, $\mathcal{O}_p(L_{max})$ and $\mathcal{O}_s(L_{max}) \neq 0$; in SF $\rho_s \neq 0$, $S(\pi) = 0$, $\Delta_c = \Delta_n = 0$, $\mathcal{O}_p(L_{max}) = \mathcal{O}_s(L_{max}) = 0$; in HI, $\rho_s = 0$, $S(\pi) = 0$, Δ_c and $\Delta_n \neq 0$, $\mathcal{O}_p(L_{max}) = 0$, $\mathcal{O}_s(L_{max}) \neq 0$. In the SS phase, CDW and SF order coexist and one expects $\rho_s \neq 0$, $S(\pi) \neq 0$, $\Delta_c = \Delta_n = 0$ and, because $S(\pi) \neq 0$, $\mathcal{O}_p(L_{max}) \neq 0$, $\mathcal{O}_s(L_{max}) \neq 0$. The gaps, Δ_c and Δ_n behave in a subtle way in the CDW and HI phases (see below).

We start with the system at $\rho = 1$ and study the phases as functions of t/U. Figure 1 shows the dependence on t/U of ρ_s, $S(k = \pi)$, $\mathcal{O}_s$, $\mathcal{O}_p$, Δ_c and Δ_n. Figure 1(c) shows that in the CDW phase $\Delta_c > \Delta_n$ and that $\Delta_n = 0$, $\Delta_c \neq 0$ at the CDW-HI transition. The HI-SF transition is signaled by $\Delta_c = \Delta_n \to 0$ [19, 20]. Finite size scaling of the DMRG results show that $\Delta_n \to 0$ at $t/U \approx 0.32 \pm 0.01$. Therefore, according to the criteria discussed above, the system is in the CDW phase for $t/U \leq 0.22$ and in the SF phase for $t/U \geq 0.32$. For $0.22 \leq t/U \leq 0.32$ (between the two vertical dashed lines), the system is in the HI phase with $\rho_s \to 0$ as the size increases. Note how slowly $\rho_s \to 0$ with increasing L and how insensitive $\mathcal{O}_s$ is to the finite size. This makes $\mathcal{O}_s$ a more reliable indicator at moderate system sizes. Our CDW-HI transition at $t/U = 0.22$ agrees very well with Fig. 1 in [26]. However, the value we obtain for the HI-SF transition, $t/U \approx 0.32$ does not agree with the schematic dashed line in that figure.

As mentioned above, the behavior at $\rho = 1$ may be understood by making the analogy with $S = 1$ spin chains. The question arises then as to whether such an analogy between this extended BHM at $\rho = 2, 3\ldots$ and $S = 2, 3\ldots$ spin chains is valid and also leads to HI phases. This question is addressed in Fig. 2 for $\rho = 2$ which shows qualitatively different behavior compared to Fig. 1. While for low t/U both cases exhibit CDW phases, the behavior of Δ_c and Δ_n, calculated with DMRG, is strikingly different as seen in Fig. 2(c): For $\rho = 2$, $\Delta_c = \Delta_n$ and finite size scaling shows that they vanish together at $t/U \approx 0.36$, which indicates that there is no HI in this case. This is consistent with the absence of the Haldane phase in $S = 2$ spin chains [35]. Nonetheless, for this filling, the system does exhibit another salient feature: Indeed, figure 2(a) and (c) show from both QMC and DMRG that when the gaps vanish, $S(\pi)$ remains non-zero while ρ_s also takes a non-zero value. $S(\pi)$ and ρ_s both remain non-zero for $0.33 \leq t/U \leq 0.425$ indicating the presence of a supersolid phase. The CDW-SS transition is estimated to be at $t/U \approx 0.33$ from QMC and $t/U \approx 0.36$ from DMRG while both DMRG and QMC give $t/U \approx 0.425$ for the SS-SF transition. In Fig. 4 we show n_k/L and $S(k)$ in the SS phase at $t/U = 0.35$ and $L = 64, 100, 128$. We see that while $n_k/L \to 0$ (see center peak, $k = 0$) as expected (since there is no condensate in one dimension), the peaks in $S(k)$ do not depend on L, indicating long range CDW order. This behavior is also confirmed by a finite-size scaling analysis of the DMRG results for sizes $L = 64, 96, 128, 160$. For the three phases (CDW, SS and SF), the CDW order parameter $S(\pi)$ is found to scale as $S_0 + S_1/L + S_2/L^2$, whereas n_0/L is always found to decay as a power law n_1/L^α. More precisely, one obtains the following results: for $t/U = 0.25$ (CDW): $S_0 = 3.4$ and $\alpha \approx 0.95$; for $t/U = 0.39$ (SS): $S_0 = 1.6$ and $\alpha \approx 0.22$; for $t/U = 0.49$ (SF): $S_0 \approx 0$ and $\alpha \approx 0.14$. Note that, in both SS and SF phases, the parameter α is less than 0.25, in agreement with a Luttinger liquid description of the system [19, 20, 27, 28]. This scaling law and the insensitivity of ρ_s to L, Fig. 2(a), confirm that this is indeed the SS phase. This surprising appearance of the SS phase at commensurate filling has also been observed in two and three dimensions [17, 18]. Furthermore, we find that the Green function, $G(r) = \langle a_r^\dagger a_0 \rangle$, decays as a power in the SS phase with exponent ≈ 0.5 at $t/U = 0.34$.

For the present value of V/U, this behavior at $\rho = 2$ is repeated at $\rho = 3$ (and presumably at higher integer fillings): As t/U is increased, the system goes from CDW

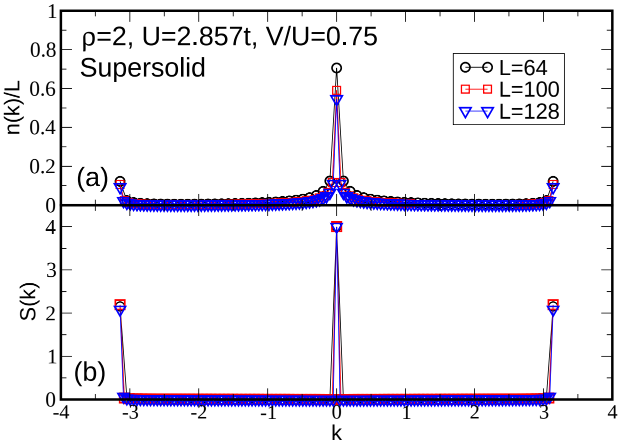

FIG. 3: (color online) The dependence of the momentum distribution, n_k/L and the structure factor,$S(k)$ on the system size. $n_k/L \to 0$ with increasing L while $S(k)$ remains constant indiating long range CDW order.

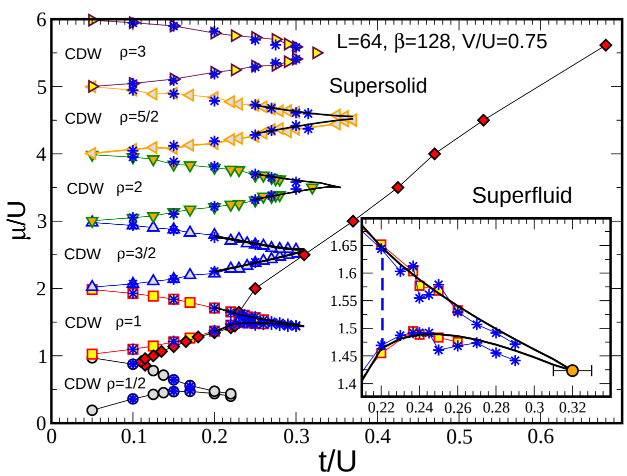

FIG. 4: (color online) Main panel: The phase diagram of the BHM obtained with QMC and DMRG simulations. All results are for a system with $V/U = 0.75$. All symbols are from QMC and are for $L = 64$ sites, $\beta = 128$ (stars are for $L = 128$). Black lines near the tips of the CDW lobes are DMRG results for $L = 192$. Inset: A zoom of the tip of the $\rho = 1$ lobe. To the right of the vertical dashed line ($t/U = 0.22$) is the HI phase, to the left is the CDW.

to SS to SF without exhibiting any HI phases. It appears, therefore, that, at least for $V/U = 3/4$, the analogy between integer spin chains and this extended BHM at integer fillings applies only at $\rho = 1$.

The phase diagram in the $(t/U, \mu/U)$ plane for $V/U = 0.75$ is mapped by calculating the charge gaps at commensurate fillings, multiples of $L/2$, and by making plots like Figs. 1, 2 which allow us to identify the various phases. We have also verified that, for incommensurate fillings, DMRG agrees with QMC on the boundary between the SS-SF. The result is shown in Fig. 4. Figure 4 was obtained using QMC (all symbols) and DMRG (black lines near lobe tips). The QMC results are for $L = 128$ (stars) and $L = 64$ (all other symbols), $\beta = 128$. The solid black lines near the lobe tips are obtained from DMRG with $L = 192$. The end points of the lobes are obtained by studying the finite size dependence of Δ_n using DMRG. The inset is a zoom of the tip of the $\rho = 1$ lobe.

Several comments are in order. The $\rho = 1/2$ lobe is surrounded almost entirely by SF except for a small region of SS squeezed between it and the $\rho = 1$ lobe. The fact that in the extended BHM a SS does not exist when the $\rho = 1/2$ CDW phase is doped with holes, but does when it is doped with particles, was already addressed in [11]. The $\rho = 1$ lobe sticks out of the SS phase and the part sticking out is, in fact, the HI phase. No other CDW lobe behaves this way. The $\rho = 3/2$ lobe terminates right at the boundary with the SF phase: To within the resolution of our simulations, the transition from the $\rho = 3/2$ CDW lobe goes directly into the SF phase without passing through the SS phase. This peculiar behavior for $\rho = 3/2$ was also observed with additional DMRG results for different values of V/U ranging from 0.65 to 1: The SS layer between the CDW and SF phases, if present, is too thin to observe for the considered system sizes. An accurate determination of the (U, V) phase diagram for this filling will require a more thorough finite size scaling analysis. All other CDW lobes, $\rho \geq 2$, are surrounded entirely by the SS phase. It is interesting to compare this figure with Fig. 3 of [17] and with the mean-field predictions [36].

In this letter we examined the phase diagram of the extended BHM at a fixed ratio of the interaction terms, $V/U = 3/4$. Contrary to expectation, we found that this model at integer fillings does not always behave analogously to integer spin chains. In particular, only for $\rho = 1$ and at small t/U does this happen and the system exhibits CDW, HI and SF phases. In the CDW phase at this filling, $\Delta_c > \Delta_n$. At all other integer fillings, we found the HI phase to be absent and in its place a supersolid phase which indicates that the system at these fillings may not behave like an integer spin chain. Furthermore, for all CDW phases, except the one at $\rho = 1$, we found that $\Delta_n = \Delta_c$ and that, unlike the $\rho = 1$ case, both gaps vanish together as the CDW phase gives way to SS or SF. It is possible that, for a different V/U ratio, the SS-SF boundary will shift and cut the $\rho = 3$ lobe (as it does in Fig. 4 with the $\rho = 1$ lobe) resulting in a HI phase. If this happens, it could mean there are two types of $\rho = 3$ CDW phases, one in which the neutral

and charge gaps are always the same (what we find here) and another CDW phase in which $\Delta_c > \Delta_n$ as is the case for the $\rho = 1$ CDW. We have also shown that the single particle Green function decays as a power law in the SS phase. Finally, from a theoretical point of view, it would be interesting to characterize the universality classes of the different quantum phase transitions (CDW-SS-SF) occuring in the system. In addition, in order to have clear experimental signatures of the phases, in particular with cold atom gases which allow time-resolved measurements one would need to study the excitations of the system.

We thank T. Giamarchi for very helpful discussions. This work was supported by: the CNRS-UC Davis EPOCAL joint research grant; by the France-Singapore Merlion program (PHC Egide and FermiCold 2.01.09); by the LIA FSQL; by an ARO Award W911NF0710576 with funds from the DARPA OLE Program and by NSF grant OISE-0952300. The Centre for Quantum Technologies is a Research Centre of Excellence funded by the Ministry of Education and National Research Foundation of Singapore.

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[37] Note that our definitions of $\mathcal{O}_p$ and $\mathcal{O}_s$ differ slightly from [19, 20] in that the sum in the exponents is done from i to j. This makes $|\mathcal{O}_p| = |\mathcal{O}_s|$ in the CDW phase for $\rho = 1$.